

Trimethyl phosphate

512-56-1 | DTXSID1021403

Model Performance

Model	Data
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Weighted KNN model

5-fold CV (75%)		Training (75%)		Test (25%)	
Q2	RMSE	R2	RMSE	R2	RMSE
0.93	22.5	0.93	22.1	0.93	22.1

Model Results

Predicted value: 185 °C

Global applicability domain: Inside

Local applicability domain index: 6.51e-01

Confidence level: 6.16e-01

Nearest Neighbors from the Training Set

<div>Image not found</div> <div>Trimethyl phosphate</div> <div>Measured: 197</div> <div>Predicted: 185</div>	<div>Image not found</div> <div>Dimethyl methylphosphonate</div> <div>Measured: 181</div> <div>Predicted: 173</div>	<div>Image not found</div> <div>Sarin</div> <div>Measured: 147</div> <div>Predicted: 156</div>
<div>Image not found</div> <div>Diethyl methanephosphonate</div> <div>Measured: 194</div> <div>Predicted: 193</div>	<div>Image not found</div> <div>Trimethyl phosphite</div> <div>Measured: 112</div> <div>Predicted: 131</div>	